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13. ABSTRACT *(Maximum 200 words)*

A physical, crystal mechanics-based theory of thermo-elasto-viscoplasticity which is valid for large strains and high strain rates at low homologous temperatures has been formulated. The theory is able to predict the macroscopic anisotropic stress-strain response, the evolution of crystallographic texture, and the macroscopic shape changes for bcc tantalum. The material functions and parameters in the model were determined by calibrating the model against existing experimental results for tantalum. The model reproduces the data of these researchers rather well. The constitutive model has been implemented in the finite element program ABAQUS Explicit by writing a "user material" subroutine. The ability of the constitutive model and computational procedures to capture the effect of initial texture on the final shape under high strain rates and large strains was evaluated by carrying out a simulation of a Taylor rod-impact experiment and by comparing the predicted final shape to that observed experimentally.

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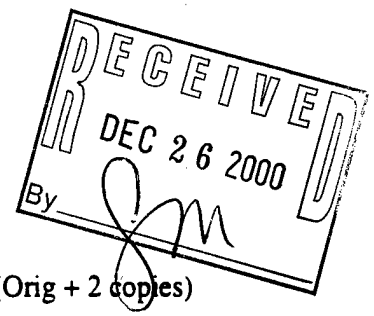

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Sincerely,

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FINAL PROGRESS REPORT

Grant Title: **Large Deformation Plasticity of Polycrystalline Tantalum**
Grant Number: DAA04-94-G-0060
Principal Investigator: Lallit Anand
Name of Institution: Massachusetts Institute of Technology

1. **Statement of Problem Studied:**

   Tantalum is a high-density, high-ductility bcc material of interest to the ARMY as a possible liner material for explosively-formed penetrators (EFPs). An important issue in the design of the liners for EFPs is the role of the initial texture of the liner in the evolution of the macroscopic shape during the process of liner collapse. A prerequisite for developing a computational capability to simulate the evolution of the macroscopic shape of an EFP is a physical, crystal mechanics-based theory of thermo-elasto-viscoplasticity which is valid for large strains ($\approx 300 - 500\%$) and high strain rates (up to $\approx 10^6 \text{sec}^{-1}$) at low (< 0.5) homologous temperatures. The theory should be able to predict the macroscopic anisotropic stress-strain response, the evolution of crystallographic texture, and the macroscopic shape changes for bcc tantalum.

   The major thrust in our research over the period of the grant was modeling of high rate deformation of b.c.c. tantalum using crystal plasticity models.

   In addition we conducted research on modeling of inelastic deformation of f.c.c. metals due to slip and twinning.

2. **Summary of Most Important Results:**

   The scientific progress in both areas is briefly summarized below:

   (a) **TANTALUM:**

   i. Strain-rate and temperature-dependent constitutive equations for polycrystalline metals which are capable of modeling the initial and evolving anisotropy in ductile metallic materials due to the evolution of crystallographic texture were formulated and then specialized to reproduce the stress-strain response of commercially pure b.c.c. tantalum for strains up to 60%, at strain rates from quasi-static to $30{,}000\,\text{s}^{-1}$, and temperatures from -200 to 525°C.

   ii. The constitutive equations were implemented in a finite element program.

   iii. The computational capability was used to simulate the evolution of crystallographic texture in simple compression, plane-strain compression and torsion under quasi-static conditions.

A comparison of the predictions against corresponding experiments showed that the crystal plasticity-based model predicts the texture evolution and the macroscopic stress-strain curves satisfactorily.

iv. The computational capability was also used to simulate the dynamic Taylor rod-impact tests on pre-textured tantalum cylinders.
The numerical simulations were shown to reasonably reproduce the final length and the ovalized macroscopic shape of the impact end of the cylinders observed in experiments.

(b) **CRYSTAL PLASTICITY BY COMBINED SLIP AND TWINNING**

There have been considerable recent advances in the understanding of anisotropy due to crystallographic texturing, and a reasonably successful elasto-viscoplasticity theory for the deformation of face-centered-cubic (f.c.c) single crystals and polycrystals with high stacking fault energies is now at hand. The high stacking fault energy f.c.c. materials (e.g. Cu, Al) deform predominantly by crystallographic slip. In contrast, for materials with low stacking energies (e.g. α-brass), in addition to crystallographic slip, *deformation twinning* plays an important role in maintaining generalized plastic flow. A direct manifestation of twinning is the different crystallographic texture that is observed in 70-30 brass as compared to pure copper.

In our research

i. We formulated an incremental constitutive model which accounts for both slip and twinning. Since twinning occurs very rapidly, and visco-plastic models of twinning are nebulous, we developed a *rate-independent* crystal plasticity model to account for slip and twinning, and also developed a new scheme to determine the active systems and the shear increments on the active slip and twin systems.

ii. We implemented our constitutive equations in the finite-element program ABAQUS/Explicit.

iii. By using comparisons between model predictions and macroscopically-measured stress-strain curves and texture evolution we deduced information about the values of the single-crystal parameters associated with slip and twin system deformation resistances and hardening due to slip and twinning.

iv. We showed that our model was able to reproduce both the experimentally measured pole figures and the stress-strain curves in plane strain compression for α-brass.

v. With the model so calibrated, we showed that the predictions for the texture and stress-strain curves from the model were also in reasonably good agreement with experiments in simple compression.

vi. We also evaluated the applicability of a Taylor-type model for combined slip and twinning.

Our calculations showed that for the high-symmetry f.c.c. brass, a Taylor-type model for crystals deforming by combined slip and twinning is able to reasonably well predict the macroscopic stress-strain curves and crystallographic texture evolution.

vii. Our calculations showed that in plane strain as well as simple compression, the crystallographic texture that develops is a result of lattice rotation due to both slip and twinning, and that in contrast to copper which does not twin under normal circumstances, it is twinning which is responsible for the brass-type texture that is observed in f.c.c. metals with low stacking fault energies.

3. LIST OF PUBLICATIONS

(a) Papers in peer-reviewed journals:

i. Kothari, M., and Anand, L.,"Elasto-Viscoplastic Constitutive Equations For Polycrystalline Metals: Application To Tantalum," *Journal of the Mechanics and Physics of Solids*, **46**, pp. 51-83, 1998.

ii. Staroselsky, A., and Anand, L.,"Inelastic Deformation Of Polycrystalline Face Centered Cubic Materials By Slip and Twinning," *Journal of the Mechanics and Physics of Solids*, **46**, pp. 671-696, 1998.

iii. Anand, L., and Kothari, M.,"A Computational Procedure For Rate Independent Crystal Plasticity," *Journal of the Mechanics and Physics of Solids*, **44**, pp. 525-558, 1996.

(b) Book Chapters:

i. Anand, L., Balasubramanian, S., and Kothari, M.,"Constitutive Modeling Of Polycrystalline Metals at Large Strains: Application To Deformation Processing," in *Large Plastic Deformation of Crystalline Aggregates*, CISM 376, Springer, New York, 1997, pp. 109– 172.

ii. Staroselsky, A., and Anand, L.,"Inelastic Deformation of F.C.C. Single Crystals by Slip and Twinning," in *Material Instabilities in Solids*, Edited by Rene de Borst and Erik van der Giessen, John Wiley, 1998, pp. 227-242.

(c) Paper in conference proceedings:

i. "Large Deformation Plasticity of F.C.C. Metals Due To Slip and Twinning," Proceedings of International Conference on *Displacive Phase Transformations and Their Applications in Materials Engineering*, held March 8 and 9, 1996, at the University of Illinois, Urbana.

4. **SCIENTIFIC PERSONNEL**

(a) Mr. Manish Kothari. Completed Ph.D. Now at Schlumberger Research.

(b) Mr. Alexander Staroselsky. Completed Ph.D. Now at United Technologies Research Center.

5. **INVENTIONS** None.